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6. AUTHORS

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14. ABSTRACT

Challenges addressed under the grant include: (i) improving our understanding of the many-electron quantum mechanisms by which nature uses strong electron correlation for efficient energy transfer, particularly in photosynthesis and bioluminescence, (ii) providing an innovative paradigm for energy transfer in photovoltaic materials by which new levels of solar efficiency are achieved through the use of strong electron correlation and entanglement, (iii) enhancing two-electron reduced-density-matrix (2-RDM)-based electronic-structure methods that significantly expand the range of strongly correlated molecular systems that can be studied with applications

15. SUBJECT TERMS

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Report Title

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ABSTRACT

Challenges addressed under the grant include: (i) improving our understanding of the many-electron quantum mechanisms by which nature uses strong electron correlation for efficient energy transfer, particularly in photosynthesis and bioluminescence, (ii) providing an innovative paradigm for energy transfer in photovoltaic materials by which new levels of solar efficiency are achieved through the use of strong electron correlation and entanglement, (iii) enhancing two-electron reduced-density-matrix (2-RDM)-based electronic-structure methods that significantly expand the range of strongly correlated molecular systems that can be studied with applications throughout science and engineering, and (iv) developing a new generation of large-scale, parallel algorithms for performing semidefinite programming with applications to problems in engineering, computer science, statistics, finance and economics. Research led to important technology transitions including the formation of RDMCHEM LLC, a software company that is developing the next generation of computational software for chemistry with applications to engineering, molecular biology, and physics.

Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Received	Paper
03/28/2013 15.00	Erik P. Hoy, Christine A. Schwerdtfeger, David A. Mazziotti. Relative Energies and Geometries of the cis- and trans-HO3 Radicals from the Parametric 2-Electron Density Matrix Method, The Journal of Physical Chemistry A, (02 2013): 1817. doi: 10.1021/jp3105562
03/28/2013 18.00	Christine A. Schwerdtfeger, David A. Mazziotti. Treating molecules in arbitrary spin states using the parametric two-electron reduced-density-matrix method, The Journal of Chemical Physics, (07 2012): 34107. doi: 10.1063/1.4731810
03/28/2013 17.00	David A. Mazziotti, Jonathan J. Foley. Measurement-driven reconstruction of many-particle quantum processes by semidefinite programming with application to photosynthetic light harvesting, Physical Review A, (07 2012): 12512. doi: 10.1103/PhysRevA.86.012512
03/28/2013 16.00	Andrew J. S. Valentine, David A. Mazziotti. Theoretical Prediction of the Structures and Energies of Olympicene and its Isomers, The Journal of Physical Chemistry A, (03 2013): 0. doi: 10.1021/jp312384b
03/28/2013 14.00	Andrew M. Sand, David A. Mazziotti. Parametric two-electron reduced-density-matrix method with application to diradical rectangular H4, Computational and Theoretical Chemistry, (01 2013): 44. doi: 10.1016/j.comptc.2012.09.033
03/28/2013 13.00	Christine A. Schwerdtfeger, David A. Mazziotti. Low-rank spectral expansions of two electron excitations for the acceleration of quantum chemistry calculations, The Journal of Chemical Physics, (12 2012): 244103. doi: 10.1063/1.4770278
08/31/2012 1.00	Christine A. Schwerdtfeger, David A. Mazziotti. Populations of Carbonic Acid Isomers at 210 K from a Fast Two-Electron Reduced-Density Matrix Theory, The Journal of Physical Chemistry A, (11 2011): 0. doi: 10.1021/jp2057805
08/31/2012 12.00	David A. Mazziotti. Effect of strong electron correlation on the efficiency of photosynthetic light harvesting, The Journal of Chemical Physics, (2012): 0. doi: 10.1063/1.4746244
08/31/2012 11.00	David Mazziotti. Structure of Fermionic Density Matrices: Complete N-Representability Conditions, Physical Review Letters, (06 2012): 0. doi: 10.1103/PhysRevLett.108.263002
08/31/2012 10.00	David Mazziotti. Significant conditions for the two-electron reduced density matrix from the constructive solution of N representability, Physical Review A, (06 2012): 0. doi: 10.1103/PhysRevA.85.062507
08/31/2012 9.00	A. Eugene DePrince, David A. Mazziotti. Connection of an elementary class of parametric two-electron reduced-density-matrix methods to the coupled electron-pair approximations, Molecular Physics, (06 2012): 0. doi: 10.1080/00268976.2012.695027
08/31/2012 8.00	Christine A. Schwerdtfeger, David A. Mazziotti, Andrew M. Sand. Strongly correlated barriers to rotation from parametric two-electron reduced-density-matrix methods in application to the isomerization of diazene, The Journal of Chemical Physics, (2012): 0. doi: 10.1063/1.3675683
08/31/2012 7.00	Christine A. Schwerdtfeger, David A. Mazziotti, Erik P. Hoy. Isoelectronic analogue of oxywater: a parametric two-electron reduced-density-matrix study of ammonia oxide, Molecular Physics, (05 2012): 0. doi: 10.1080/00268976.2012.668226

08/31/2012 6.00 David A. Mazziotti. Two-Electron Reduced Density Matrix as the Basic Variable in Many-Electron Quantum Chemistry and Physics,
Chemical Reviews, (01 2012): 0. doi: 10.1021/cr2000493

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The Journal of Physical Chemistry A, (12 2011): 0. doi: 10.1021/jp208013m

08/31/2012 3.00 David A. Mazziotti, Nolan Skochdopole. Functional Subsystems and Quantum Redundancy in Photosynthetic Light Harvesting,
The Journal of Physical Chemistry Letters, (12 2011): 0. doi: 10.1021/jz201154t

08/31/2012 2.00 Nathania Hau, David Mazziotti, Kasra Naftchi-Ardebili. Rank restriction for the variational calculation of two-electron reduced density matrices of many-electron atoms and molecules,
Physical Review A, (11 2011): 0. doi: 10.1103/PhysRevA.84.052506

08/31/2013 19.00 Jonathan J. Foley, David A. Mazziotti. Cage versus Prism: Electronic Energies of the Water Hexamer,
The Journal of Physical Chemistry A, (08 2013): 0. doi: 10.1021/jp405739d

08/31/2013 20.00 Erik P. Hoy, Neil Shenvi, David A. Mazziotti. Comparison of low-rank tensor expansions for the acceleration of quantum chemistry computations,
The Journal of Chemical Physics, (07 2013): 34105. doi: 10.1063/1.4813495

09/24/2014 21.00 Andrew M. Sand, Claire Liu, Andrew J. S. Valentine, David A. Mazziotti. Modulating the Electronic Structure of Chromophores by Chemical Substituents for Efficient Energy Transfer: Application to Fluorone,
The Journal of Physical Chemistry A, (07 2014): 0. doi: 10.1021/jp503900m

09/24/2014 22.00 Luke W. Bertels, David A. Mazziotti. Accurate prediction of diradical chemistry from a single-reference density-matrix method: Model application to the bicyclobutane to gauche-1,3-butadiene isomerization,
The Journal of Chemical Physics, (07 2014): 0. doi: 10.1063/1.4890117

09/24/2014 23.00 Nicholas C. Rubin, David A. Mazziotti. Comparison of one-dimensional and quasi-one-dimensional Hubbard models from the variational two-electron reduced-density-matrix method,
Theoretical Chemistry Accounts, (5 2014): 0. doi: 10.1007/s00214-014-1492-7

09/24/2014 24.00 Romit Chakraborty, David A. Mazziotti. Generalized Pauli conditions on the spectra of one-electron reduced density matrices of atoms and molecules,
Physical Review A, (4 2014): 0. doi: 10.1103/PhysRevA.89.042505

09/24/2014 25.00 Srikant Veeraraghavan, David A. Mazziotti. Global solutions of restricted open-shell Hartree-Fock theory from semidefinite programming with applications to strongly correlated quantum systems,
The Journal of Chemical Physics, (03 2014): 0. doi: 10.1063/1.4868242

09/24/2014 26.00 Srikant Veeraraghavan, David A. Mazziotti. Global solutions of Hartree-Fock theory and their consequences for strongly correlated quantum systems,
Physical Review A, (1 2014): 0. doi: 10.1103/PhysRevA.89.010502

09/24/2014 27.00 Gergely Gidofalvi, David A. Mazziotti. Molecule-Optimized Basis Sets and Hamiltonians for Accelerated Electronic Structure Calculations of Atoms and Molecules,
The Journal of Physical Chemistry A, (01 2014): 0. doi: 10.1021/jp410191y

09/24/2014 28.00 Julie T. Skolnik, David A. Mazziotti. Cumulant reduced density matrices as measures of statistical dependence and entanglement between electronic quantum domains with application to photosynthetic light harvesting,
Physical Review A, (9 2013): 0. doi: 10.1103/PhysRevA.88.032517

TOTAL: **28**

Number of Papers published in peer-reviewed journals:

(b) Papers published in non-peer-reviewed journals (N/A for none)

Received Paper

TOTAL:

Number of Papers published in non peer-reviewed journals:

(c) Presentations

Number of Presentations: 0.00

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Received Paper

TOTAL:

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Received Paper

TOTAL:

Number of Manuscripts:

Books

Received Book

TOTAL:

Received Book Chapter

TOTAL:

Patents Submitted

Patents Awarded

Awards

2012: Promotion of PI to Full Professor at The University of Chicago

2014: Quantrell Award to PI from The University of Chicago

2014: Semifinalist Intel Science Talent Search Award to Claire Liu

2014: NSF Graduate Fellowship to Luke Bertels

2014: NSF Graduate Fellowship to Andrew Valentine

Graduate Students

NAME	PERCENT_SUPPORTED	Discipline
Andrew Sand	0.20	
Erik Hoy	0.20	
Nick Rubin	0.20	
Srikent Vera Rhaghavan	0.20	
Andrew Valentine	0.20	
Charles Forgy	0.20	
Erica Sturm	0.20	
Romit Chakraborty	0.20	
Christine Schwerdtfeger	0.20	
Jay Foley	0.20	
FTE Equivalent:	**2.00**	
Total Number:	**10**	

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
David A. Mazziotti	0.08	
FTE Equivalent:	**0.08**	
Total Number:	**1**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED	Discipline
Luke Bertels	0.50	Chemistry
Nolan Skochdopole	0.30	Chemistry
Claire Liu	0.50	Chemistry
Kasra Naftchi-Ardebili	0.30	Chemistry
James Snyder	0.30	Chemistry
FTE Equivalent:	**1.90**	
Total Number:	**5**	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	4.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:	4.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:	4.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):	4.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	3.00

Names of Personnel receiving masters degrees

NAME
Total Number:

Names of personnel receiving PHDs

NAME
Jay Foley (0.2)
Srikant Vera Rhaghavan (0.2)
Total Number: 2

Names of other research staff

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Sub Contractors (DD882)

Inventions (DD882)

Scientific Progress

See Attachment

Technology Transfer

Areas of technology transfer include:

(1) Formation of a start-up company RDMCHEM LLC in 2014. RDMCHEM LLC is a software company that is developing the next generation of computational software for chemistry with applications to engineering, molecular biology, and physics.

(2) Distribution of software: The ARO grant led to the production of a research code that is distributed at http://mazziotti.uchicago.edu.

(3) The grant supported research by my graduate student Jonathan Foley who is currently on staff at Argonne National Laboratory.

(4) The grant supported research by my graduate student Loren Greenman who is currently a postdoctoral fellow at Berkeley National Laboratory.

(5) The grant supported the undergraduate student Luke Bertels and my graduate student Andrew Valentine who received 2014 graduate fellowships from the National Science Foundation.

(6) The grant supported the high school student Claire Liu who was named a semifinalist in the 2014 Intel Science Talent Search for her ARO-sponsored research.

Final Report 2014

David A. Mazziotti
The University of Chicago

Statement of the Problem Solved

Challenges addressed by the research include: (i) improving our understanding of the *many-electron quantum mechanisms* by which nature uses strong electron correlation for efficient energy transfer, particularly in photosynthesis and bioluminescence, (ii) providing an innovative *paradigm for energy transfer in photovoltaic materials* by which new levels of solar efficiency are achieved through the use of strong electron correlation and entanglement, (iii) enhancing two-electron reduced-density-matrix (2-RDM)-based electronic-structure methods that significantly expand the range of strongly correlated molecular systems that can be studied with applications throughout science and engineering, and (iv) developing a new generation of large-scale, parallel algorithms for performing semidefinite programming with applications to problems in engineering, computer science, statistics, finance and economics.

Summary of the Most Important Results

Significant research was supported under a prior grant from the Army Research Office. The research produced 33 published papers[1-33] and partially supported the training of 12 graduate students, 5 undergraduate students, and 1 high school student. The high school student Claire Liu was recently named one of the semifinalists in the 2014 Intel Science Talent Search for her research project, "The Effect of Electron Correlation on Efficient Energy Transfer in a Synthetic Chromophore System." Highlights of the research include:

1) Development, Application, and Distribution of the Parametric 2-RDM Method: Under the ARO grant we developed the parametric 2-RDM method (p2-RDM) in which the 2-RDM is parameterized by single and double excitations. The p2-RDM method has a smaller pre-factor in its computational scaling than coupled cluster singles-doubles with an accuracy approaching wave function methods with triple excitations, especially in the presence of multi-reference correlation. Applications have been made to strongly correlated transition states and intermediates including the rotational transition state between the *cis* and *trans* diazene as well as the diradical isomers of the recently discovered olympicene molecule. The method has also been applied to showing the importance of multi-reference correlation on small energy differences which arise in determining the existence and stability of oxywater and the relative energies and stability of the cage and prism isomers of water hexamer. The p2-RDM method has made available for download from the research group's website.

2) Prototype Low-scaling 2-RDM Method: Using tensor factorizations of the double-excitation and Hamiltonian matrices, we developed a prototype, low-scaling 2-RDM method that scales computationally as $O(r^4)$ where r is the number of orbitals in the one electron basis set. Further development of the method has the potential to provide an *ab initio* alternative to density functional theory.

3) Complete Set of N-representability Conditions: The 2-RDM must be constrained for its two electrons to represent an N-electron quantum system. These constraints are known as N-representability conditions. With ARO support we presented a constructive solution to the N-representability problem: a full characterization of the conditions for constraining the two-

electron reduced density matrix to represent an *N*-electron density matrix. Previously known conditions, while rigorous, were incomplete. We derived a hierarchy of constraints built upon (i) the bipolar theorem and (ii) tensor decompositions of model Hamiltonians. Existing conditions (D, Q, G, T1, and T2), known classical conditions, and new conditions appear naturally. This theoretical advance gives completeness to the foundation of 2-RDM quantum theory. Conditions beyond T2 will eventually allow for the computation of molecular quantum systems in polynomial time with unprecedented accuracy.

4***) Efficient Algorithm for Large-scale Semidefinite Programming:*** We developed a more efficient approach to adding *N*-representability conditions to 2-RDM calculations based on a boundary-point algorithm for semidefinite programming. The current parallel version of the boundary-point algorithm is 100 to 1000 times faster than a previous first-order algorithm for semidefinite programming developed by our group for electronic structure calculations. The algorithm has been adopted by others for 2-RDM calculations as well as other applications in science and engineering.

5) Functional Subsystems in Photosynthetic Light Harvesting: The Fenna-Matthews-Olson (FMO) antennae complex, responsible for light harvesting in green sulfur bacteria, consists of three monomers, each with seven chromophores. Skochdopole and Mazziotti showed that multiple subsystems of the seven chromophores can transfer energy from either chromophore 1 or 6 to the reaction center with an efficiency matching or in many cases exceeding that of the full seven chromophore system. In the FMO complex, these functional subsystems support multiple quantum pathways for efficient energy transfer that provide a built-in quantum redundancy. There are many instances of redundancy in nature, providing reliability and protection, and in photosynthetic light harvesting this quantum redundancy provides protection against the temporary or permanent loss of one or more chromophores. The complete characterization of functional subsystems within the FMO complex offers a detailed map of the energy flow within the FMO complex, which has potential applications to the design of more efficient photovoltaic devices.

6) Strong Correlation in Light Harvesting: We generalized the single-electron/exciton models to a multi-electron/exciton model that explicitly shows the effects of enhanced electron correlation within chromophores on the efficiency of energy transfer. Importantly, within the model the addition of electron correlation within the chromophore enhances energy transfer by as much as 100%.

7) Measurement-driven Reconstruction of Many-particle Quantum Processes: Quantum measurements provide a trove of information about a quantum system or process without solution of the Schrödinger equation, and in principle, the associated density matrix is a function of these measurements. Inversion of the measurements can produce an estimate of the density matrix, but this estimate may be unphysical, especially when the measurements are noisy or incomplete. We have recently developed a general approach based on semidefinite programming for reconstructing the density matrix from quantum measurements which leads naturally to nonnegative solutions, a critical attribute of physically realistic solutions. We have applied the methodology to reconstructing the time-dependent quantum process of exciton transfer in a photosynthetic light-harvesting complex. The research also has broad applications in advanced sensing and image reconstruction.

8) Metrics for Assessing Electron Correlation and Entanglement: Reliable but computable metrics for assessing the degree of electron correlation and entanglement are critical for studying strongly correlated molecules and materials. Reduced density matrices (RDMs) are

natural variables for measuring the degree of correlation between electrons. We studied the use of the 2-RDM and parts of the 2-RDM for the measurement of electron correlation and entanglement in the photosynthetic light harvesting of green-sulfur bacteria. We found that the squared Frobenius norm of the cumulant 2-RDM very accurately represents the entanglement in this complicated time-dependent process.

8) Strong Correlation in Molecular Systems and Processes: The 2-RDM methods were applied to computing the energies and properties of strongly correlated molecular systems and processes including chains (acenes) and sheets of polyaromatic hydrocarbons and the reaction of firefly luciferin in bioluminescence. Calculations of both ground- and excited-state energies were performed at the conical intersections in the chemiluminescence of dioxetanone and the photoexcited tautomerization of vinyl alcohol to acetylaldehyde.

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5. *Solving the Schrödinger Equation: Has Everything Been Tried?* Paul Popelier, Ed.; Imperial College Press: London, 2011. D. A. Mazziotti, Chapter 4, pp. 61-90. "Reduced-Density-Matrix Theory for Many-electron Correlation"
6. K. Naftchi-Ardebili, N. W. Hau, and D. A. Mazziotti, "Rank Restriction for the Variational Calculation of Two-electron Reduced Density Matrices of Many-electron Atoms and Molecules," *Physical Review A* **84**, 052506 (2011).
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27. S. Veeraraghavan and D. A. Mazziotti, "Global solutions of Hartree-Fock theory and their consequences for strongly correlated quantum systems," *Physical Review A* **89**, 010502 (2014).

28. L. W. Bertels and D. A. Mazziotti, “Accurate prediction of diradical chemistry from a single-reference density-matrix method: Model application to the bicyclobutane to gauche-1,3-butadiene isomerization,” *J. Chem. Phys.* **141**, 044305 (2014).
29. N. C. Rubin and D. A. Mazziotti, “"Comparison of one-dimensional and quasi-one-dimensional Hubbard models from the variational two-electron reduced-density-matrix method,” *Theor. Chem. Acc.* **133**, 1492 (2014).
30. R. Chakraborty and D. A. Mazziotti, “"Generalized Pauli conditions on the spectra of one-electron reduced density matrices of atoms and molecules,” *Phys. Rev. A* **89**, 042505 (2014).
31. S. Veeraraghavan and D. A. Mazziotti, “Global solutions of restricted open-shell Hartree-Fock theory from semidefinite programming with applications to strongly correlated quantum systems,” *J. Chem. Phys.* **140**, 124106 (2014).
32. N. Skochdopole and D. A. Mazziotti, “Functional subsystems and strong correlation in photosynthetic light harvesting,” *Adv. Chem. Phys.* **154**, 2989 (2014).
33. A. M. Sand, C. Liu, A. J. S. Valentine, and D. A. Mazziotti, “Modulating the electronic structure of chromophores by chemical substituents for efficient energy transfer: Application to fluorone,” *J. Phys. Chem. A* **X**, X (2014).